4-(Chloromethyl)-2-ethoxy-1,3,2lambda^5-dioxaphospholan-2-one

67554-11-4 | DTXSID50791173

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 9.05e-01

Global applicability domain: Inside

Local applicability domain index: 4.82e-01

Confidence level: 6.55e-01

Nearest Neighbors from the Training Set

Image not found
Dichlorvos
Measured: 1.43
Predicted: 1.25

Image not found
Triethyl phosphate
Measured: 0.8
Predicted: 8.20e-01

Image not found
Phosphonic acid, bis(1-methylethyl) ester
Measured: 0.45
Predicted: 5.25e-01

Image not found
Sarin
Measured: 0.3
Predicted: 3.86e-01

Image not found
Tris(2-chloroethyl) phosphate
Measured: 1.44
Predicted: 1.58